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Report

May 14, 2000

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AFOSR/NL

Grant number F49620-99-1-0150

Period of Performance: 15 February 1999- 14 February 2000

Gov't Share: \$180 K

CSM Cost Share: \$75 K

1. Fiscal Section

This grant provided for the major upgrade of our experimental facility. The following items were purchased for a total of \$255 K:

1.	High Performance FT-Visible/FTIR Interferometer System, Nicolet 860 Model	\$ 77,730.08
2.	Xe-Cl Excimer Laser, Lambda Physik Compex 102 Model	\$ 53,600.00
	excimer gases	\$ 44.83
3.	Argon-Ion Laser, Coherent Co. I-300 Model	\$ 43,378.12
4.	Vibration-Isolated Optical Table, New Port Co.	\$ 9,867.54
5.	Raman Double Monochromator, 0.85 m, SPEX 1403 Model	\$ 62,500.00
	shipping	\$ 744.80
6.	Miscellaneous components integrated with FT-Interferometer and Raman systems	
	Raman Interference Filters	\$ 3,840.00
	UPS Power back-up units	\$ 1,450.00
	PC Computer for Raman System	\$ 1,835.42
Total:		\$254,990.78

2. Technical Section

We had used the Defense-University Instrumentation Program grant (F49620-99-1-0150) in the amount of \$180,000.00 together with \$75,000 of matching funds from Colorado School of Mines to purchase new equipment as well as to upgrade existing instrumentation. The list of purchased items is attached.

All instrumentation that we proposed to purchase in our request to DURIP was installed and integrated with already existing machines. Together they create the unique experimental spectroscopy and photochemistry facility for investigations of new exotic materials and reactive transient intermediates. The Argon-Ion Laser, Coherent Co. I-300 Model was integrated with the Double Monochromator, (0.85 m, SPEX Model 1403), computer, UPS, filters, and optical table to create high performance Raman spectroscopy set-up. The excimer laser is used to excite our sample for photochemical transformations or spectroscopic measurements. The FTIR-Vis spectrometer is used to record high-resolution visible/NIR absorption and emission spectra.

At present, the facility is used mainly for research on novel exotic molecules that are of interest to DARPA/AFOSR. These are polyazetes (N_x), pure nitrogen compounds that are predicted to have highly attractive properties but have never been detected and observed. The main target of this investigation is tetrahedral N_4 (tetraazatricyclo[1.1.0.0]^{2,4}butane). The molecule is predicted to be metastable and reside in the well separated by 60 kcal/mol barrier from two N_2 molecules. This makes it potentially a very attractive candidate for next generation space craft propellant. If the molecule can be made and the above quantum-chemical estimates are correct, it should be stable at room temperature and posses propulsion properties (specific impulse, etc.) matching or exceeding these of H_2/O_2 system currently used in majority of space payload launches. The main gain would be in skipping the expensive liquid helium

technology required to refrigerate liquid hydrogen and oxygen. The potential financial savings could be substantial (order of magnitude or more).

The list of pure nitrogen compounds known is very short: N_2 , N_3 radical, N_5^+ , and a few other ions. With exception of N_2 , discovered over two centuries ago all these compounds are unstable and not fully bonded or are electrically charged.

In our attempts we had used the nitrogen plasma generated by microwave or electrical discharge in gaseous N_2 to activate otherwise inert dinitrogen. The gaseous stream was quenched on a cold window (6.2 – 35 K) and resulting matrix was examined by IR and UV-Vis absorption spectroscopies. In samples prepared with $^{14}N_2$ we observe a weak infrared transition at 936.7 cm^{-1} (Fig.1, bottom). It shifts to 900.0 cm^{-1} when $^{15}N_2$ is

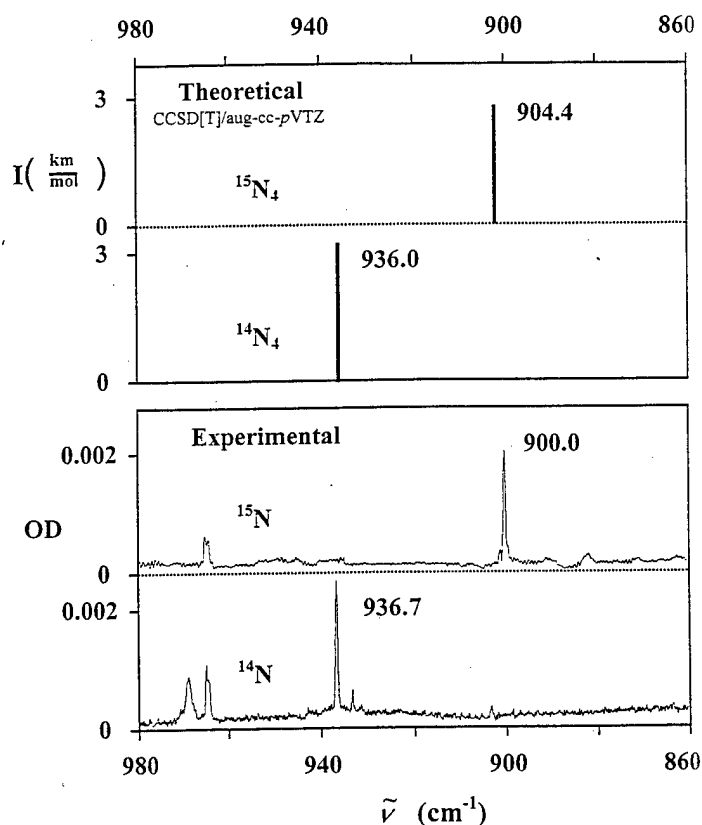


Figure 1. Observed IR absorption (lower set) from sample containing separately: $^{14}N_2$ and $^{15}N_2$ quenched plasma and respective theoretical predictions (upper set). The peak at 969 cm^{-1} (bottom spectrum) belongs to NH_3 impurity and the unresolved doublet at 965 cm^{-1} (in both spectra) originates in O_4 .

used (Fig.1, top). Both peaks do not correlate with any other absorptions in the spectra and are best explained as originating from tetrahedral tetrazetes (N_4). Their positions are compatible with quantum chemical estimates for $^{14}N_4$, at 936.0 cm^{-1} and $^{15}N_4$, at 904.4 cm^{-1} . The remainder of the recorded peaks is assigned to various nitrogen oxides or to common impurities using standard identification procedures. Although, we do not claim to have absolute proof that we prepared and indeed detected tetrazete, the experimental evidence clearly points towards such conclusion. We continue working with mixed $^{15}N^{14}N$ isotopes to record unique fingerprints of this elusive compound. We have employed various other preparation methods (i.e., fast atom or ion bombardment) and optical spectroscopy techniques (i.e., Raman and resonance Raman) to obtain independent proofs for our claims.

Most of the instrumentation provided by the DURIP grant will be also used to spectroscopically characterize N_5^- (pentazole anion) that we are trying to prepare using synthetic methods. This work is quite advanced and we expect a conclusion very soon. We will continue using this instrumentation for future research funded by DOD projects and training of undergraduate and graduate students at CSM.